Improved Error Estimate for the Valence Approximation

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We construct a systematic mean-field-improved coupling constant and quark loop expansion for corrections to the valence (quenched) approximation to vacuum expectation values in the lattice formulation of QCD. Terms in the expansion are evaluated by a combination of weak coupling perturbation theory and a Monte Carlo algorithm.

The valence (quenched) approximation to the infinite volume, continuum limit of lattice QCD gives values for hadron masses and for meson decay constants not far from experiment. Missing from these calculations, however, is an independent theoretical estimate of the error arising from the valence approximation. A possible method for determining the valence approximation's error is proposed in Ref. [1]. In the present article, we describe an improved version of of the method of Ref. [1] which we believe is likely to require less computer time. The expansion we describe can be adapted to any choice of quark action but will be given here only for Wilson quarks.

In an exact treatment of QCD, virtual quark-antiquark pairs produced by a chromoelectric field reduce the field's intensity by a factor which depends both on the field's momentum and on its intensity. In the valence approximation this factor, analogous to a dielectric constant, is approximated by its zero-field-momentum zero-field-intensity limit [2]. Our expression for the error in the valence approximation to any vacuum expectation value consists of a sum indexed by a power of a mean-field-improved coupling constant [3] and by a quark loop count. Each term in the expansion requires as input, in effect, the dielectric constant entering the valence approximation. The dielectric constant, for convenience, we obtain analytically from mean-field-improved perturbation theory to second order in the coupling constant. A related calculation without mean-field improvement is described in Ref. [4]. The remaining work of evaluating each term in the error expansion is done by a Monte Carlo algorithm.

In a simple test case, our error estimate requires significantly less computer time than a direct comparison of full QCD and the valence approximation. Whether this gain holds also for more interesting cases we do not yet know.

We consider Wilson's formulation of euclidean QCD on some finite lattice, with periodic boundary conditions for gauge links $u(x, y)$, and antiperiodic boundary conditions for the coupling matrix M for a single quark flavor. For n_f, either even or odd, degenerate flavors of quarks and any function of the gauge fields G, the vacuum expectation value obtained after integrating out quark fields is

$$
\begin{aligned}
<G> &= Z^{-1} \int d\nu \, G \, det(M)^{n_f} \, exp(\frac{\beta}{6}P), \\
Z &= \int d\nu \, det(M)^{n_f} \, exp(\frac{\beta}{6}P),
\end{aligned}
\tag{1}
$$

where, as usual, P is Wilson's plaquette action, β is $6/g^2$ for bare gauge coupling constant g, and ν is the product of one copy of $SU(3)$ Haar measure for each link variable on the lattice. We ignore for simplicity vacuum expectation values of products of quark and antiquark fields.

The valence approximation to $<G>$ of Eq. (1) is

$$
\begin{aligned}
<G>_v &= Z_v^{-1} \int d\nu \, G \, exp(\frac{\beta_v}{6}P), \\
Z_v &= \int d\nu \, exp(\frac{\beta_v}{6}P),
\end{aligned}
\tag{2}
$$

with valence approximation β_v given by $6/g_v{}^2$ for valence approximation bare gauge coupling g_v. It is convenient to define $\Delta\beta$ as the shift $\beta_v - \beta$.

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We now derive a coupling constant and quark loop expansion for the difference between a full QCD vacuum expectation value $< G >$ and its valence approximation $< G >_v$. For this purpose, we recast $< G >$ of Eq. (1) as

$$
\begin{aligned}
< G > &= Z^{-1} \int d\nu\, G\, exp(\frac{\beta_v}{6}P + Q) \\
Z &= \int d\nu\, exp(\frac{\beta_v}{6}P + Q), \qquad (3) \\
Q &= n_f tr\log(M) - \frac{\Delta\beta}{6}P,
\end{aligned}
$$

then introduce a parameter λ multiplying Q, expand $< G >$ in powers of λ, and replace λ by 1. We obtain

$$
\begin{aligned}
< G >=&< G >_v + \qquad\qquad\qquad (4) \\
&< (G- < G >_v)(Q- < Q >_v) >_v + \dots
\end{aligned}
$$

The nth term in Eq. (4) is the $n - 1$ quark loop correction to the valence approximation. As an error estimate for the valence approximation, we will concentrate on the one-loop correction $< (G- < G >_v)(Q- < Q >_v) >_v$.

For $tr\log(M)$ in the one-loop term of Eq. 4, we construct a coupling constant expansion. To do this, transform each gauge configuration to the euclidean lattice version of Landau gauge by maximizing $\sum_y tr[u(x,y)]$ at each lattice site x. One algorithm for finding this transformation is discussed in Ref. [1]. We obtain some random sample of Gribov copies the details of which play no explicit role in our expansion. For each fixed gauge configuration, let z be the average over all lattice links of $tr[u(x,y)]/3$. Let M_0 be a free hopping matrix with hopping constant κ_0 chosen to give a quark mass $1/(2\kappa_0) - 4$ that agrees with a mean-field-improved [3] value of the quark mass $1/(2z\kappa) - 1/(2z\kappa_c)$ carried by M, where κ and κ_c are, respectively, the hopping constant of M and the valence approximation to the critical value of this hopping constant.

We now express $tr\log(M)$ in the form

$$
\begin{aligned}
tr\log(M) =& \\
& tr\log\{zM_0[1 - M_0^{-1}(M_0 - z^{-1}M)]\}, \qquad (5)
\end{aligned}
$$

and expand to obtain a sum indexed, in effect, by powers of a mean-field-improved quark coupling constant [3]

$$
\begin{aligned}
tr\log(M) =& tr\log(zM_0)- \qquad\qquad\qquad (6) \\
& \sum_n \frac{1}{n} tr\{[M_0^{-1}(M_0 - z^{-1}M)]^n\}.
\end{aligned}
$$

The trace required in the second term of Eq. (6) we obtain from an ensemble of complex-valued quark fields ϕ^r, $1 \leq r \leq R$ with each component of each field an independent random complex number on the unit circle. We obtain

$$
\begin{aligned}
tr\log(M) =& tr\log(zM_0)- \qquad\qquad\qquad (7) \\
& R^{-1} \sum_{nr} \frac{1}{n} < \phi^r|[M_0^{-1}(M_0 - z^{-1}M)]^n\phi^r >,
\end{aligned}
$$

where $< \dots | \dots >$ is the inner product on the space of complex-valued quark fields. The term $tr\log(zM_0)$ in Eq. (7) can be computed by diagonalizing M_0 in momentum space, and multiplication by M_0^{-1} can be done efficiently using fast Fourier transformations.

Combining Eqs. (4) and (7) gives a coupling constant and quark-loop expansion for corrections to valence approximation vacuum expectation values. Still to be determined is the shift $\Delta\beta$. Eqs. (4) and (7) are formally correct for any choice of $\Delta\beta$. The rate at which these expansions converge, however, will be affected by the choice of $\Delta\beta$. One possible way to choose $\Delta\beta$ is to require the error or some approximation to the error in a particular physical quantity to be zero. For the present discussion, we choose $\Delta\beta$ by requiring that (analytic) mean-field-improved perturbation theory give zero valence approximation error, to first order in quark loops and second order in the coupling constant, for the Landau gauge gluon propagator at minimal nonzero momentum. We obtain

$$
\begin{aligned}
\Delta\beta &= \frac{9n_f}{4\sin^2(\pi/L) < trU >_v} \times \\
& [\Pi_{22}(p) - \Pi_{22}(0)] \qquad\qquad (8) \\
\Pi_{\mu\nu}(p) &= \frac{1}{L^4} \sum_q tr[\Gamma_\mu(q + p/2)S(q + p) \times \\
& \Gamma_\nu(q + p/2)S(q)],
\end{aligned}
$$

where L is the lattice period, p is a momentum vector with a single nonzero component p_1 of

$2\pi/L$, $< trU >_v$ is the valence approximation plaquette expectation value, and each component of q in the sum over q ranges from π/L to $2\pi - \pi/L$ in steps of $2\pi/L$. The propagator $S(q)$ has inverse $S(q)^{-1}$ of $1/(2\kappa_0) - i\sum_\mu \gamma_\mu sin(q_\mu) - \sum_\mu cos(q_\mu)$, and the vertex $\Gamma_\mu(q)$ is $sin(q_\mu) - i\gamma_\mu cos(q_\mu)$. The limiting value of $\Delta\beta$ for large L without mean-field improvement has been derived in Ref. [4].

As a test of our method we compared valence approximation expectations $< G >_v$, Eq. (2), their one-loop errors $< (G - < G >_v)(Q - < Q >_v) >_v$, Eq. (4), and the corresponding full QCD expectations $< G >$, Eq. (1), for a lattice 10^4 with β_v of 5.679, κ of 0.16 and n_f of 2. According to Eq. (8), $\Delta\beta$ is then 0.243 giving a full QCD β of 5.436. For this case $\Delta\beta$ found by the method of Ref. [1] is 0.244(6). We used 224 independent equilibrium gauge configuration in the valence approximation ensemble, generated by an over-relaxed pseudo heat bath algorithm, 600 random fermion fields R to evaluate the trace in Eq. (7) and 176 weakly correlated equilibrium gauge configurations for the full QCD ensemble, generated by a red-black preconditioned hybrid Monte Carlo algorithm. The expansion in Eq. (7) was carried to order n of 10. The calculation of $< (G - < G >_v)(Q - < Q >_v) >_v$ was not turned carefully. In particular R of 600 in Eq. (7) is much larger than its optimal vaule. The time required for the valence approximation and error calculation was still less than 5% of the time required by the full QCD calculations.

For G we used Wilson loops $W_0, \ldots W_{10}$ consisting, respectively, of paths 1×1, 2×1, all rotations of steps in the directions $\hat{1}, \hat{2}, \hat{3}, -\hat{1}, -\hat{2}, -\hat{3}$, all rotations of steps in the directions $\hat{1}, \hat{2}, \hat{3}, -\hat{2}, -\hat{1}, -\hat{3}$, 3×1, 2×2, 4×1, 5×1, 3×2, 4×2, and 3×3. For all loops, we found that the predicted error $< (W_i - < W_i >_v)(Q - < Q >_v) >_v$ converges as a function of the highest power n of coupling strength used in Eq. (7) by n of 7 or smaller. For n of 7, Fig. 1 shows the relative shift of the valence approximation from full QCD $(< W_i > - < W_i >_v)/ < W_i >$ and the predicted value $< (W_i - < W_i >_v)(Q - < Q >_v) >_v / < W_i >$. To within statistical uncertainties, the predicted errors agree with the true errors.
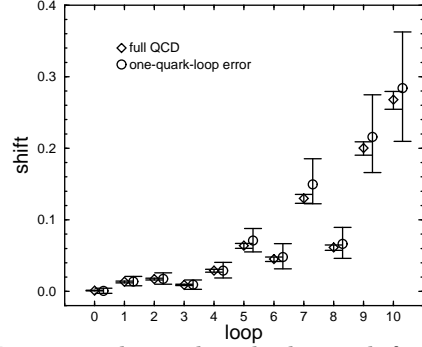

Figure 1. The predicted relative shift of 11 Wilson loops from their valence approximation values in comparison to the true shift of full QCD.

The true errors in Fig. 1 were found from the shortest full QCD run sufficient to confirm equilibration of $< W_0 >, \ldots < W_{10} >$. Nonetheless the statistical uncertainties in the predicted errors are much larger than those in the true errors. If we were to run the error prediction algorithm long enough to obtain statistical uncertainties comparable to the uncertainties found by a direct comparison of full QCD and the valence approximation, it is possible that the computer time required by the error algorithm would become comparable to that for full QCD. To find the uncertainty arising from use of the valence approximation, however, the statistical uncertainty in the error estimate does not need to be too much smaller than the error estimate's central value. Used in this way, for the set of parameters of the test, our algorithm takes significantly less time than the shortest possible direct comparison of the valence approximation and full QCD.

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